Relativistic Hartree-Fock Calculations of K-Shell Ionization Probabilities in Beta Decay

AUTHOR(S):

Mukoyama, Takeshi; Kagawa, Takashi

Bull. Inst. Chem. Res., Kyoto Univ., Vol. 61, No. 1, 1983

Relativistic Hartree-Fock Calculations of K-Shell Ionization Probabilities in Beta Decay

Takeshi MUKOYAMA* and Takashi KAGAWA†

Received January 18, 1983

The K-shell ionization probabilities in β^- decay have been calculated for ^{185}W and ^{203}Hg using the relativistic Hartree-Fock wave functions. The effect of the indistinguishability of two electrons in the final state is taken into consideration. The calculated results are compared with the experimental data and other theoretical predictions.

KEY WORDS: K-shell ionization probability/ Beta decay/ Relativistic Hartree-Fock wave function/

I. INTRODUCTION

The β^- decay is ordinally considered as a pure nuclear process due to the weak interaction by which a β particle and an antineutrino are emitted simultaneously. However, the atomic nucleus is in general surrounded by orbital electrons and there is a small probability that these electrons take part in the nuclear process. This is well known as one of the higher-order processes in nuclear β decay and takes place by three different mechanisms; excitation (shakeup) and ionization (shakeoff) of atomic electrons due to rearrangement of the electron clound caused by the sudden change in nuclear charge, and ionization of the atomic electron by the Coulomb interaction between β particle and the orbital electron (direct collision).

Since the first theoretical prediction of this process by Feinberg[1] and Migdal[2] in 1941, many theoretical and expreimental studies have been reported.[3] Especially in recent years a large amount of the experiments have been made for K-shell vacancy production probabilities in β^- decay. It is believed that the most dominant mechanism for K-vacancy production accompanying β^- decay is the shakeoff process and that other mechanisms play a minor role. However, comparison of the recent experimental data with the theoretical predictions for the K-shell shakeoff probabilities with the relativistic hydrogenic wave functions has shown that the theory underpredicts the experimental values.[4]

We have pointed out[5] that the existence of other electrons in the atom increases the K-shell ionization probabilities and improves the agreement between theory and experiment. This is due to reduction of the effective nuclear charge seen by the K-shell electron concerned. The calculations have been made using the K-shell wave functions in the complex atom proposed by Greenland and Irvine.[6] This model has

* 向山 毅: Laboratory of Nuclear Radiation, Institute for Chemical Research, Kyoto University, Kyoto. 606

† 香川貴司: Department of Physics, Nara Women's University, Nara. 630.

been extended to include the effect of the indistinguishability between two electrons in the final continuum state (β^- particle and emitted K-shell electron).[7] The calculated results agree well with the hydrogenic model corrected for the many-electron effect,[4] but are systematically smaller than the recent experimental data. This means that there still remains the discrepancy between theory and experiment.

It should be noted, however, that the K-shell shakeoff process arises from the imperfect-wave-function overlap between the initial and final atomic states and is very sensitive to the choice of atomic wave functions. The Greenland-Irvine (G-I) wave function is an approximate wave function based on the nonrelativistic Hartree-Fock-Slater calculations of Herman and Skillman.[8] It is desirable to perform calculations for K-shell ionization probabilities in β^- decay using more realistic wave functions.

In the present work, the K-electron shakeoff probabilities accompanying β^- decay have been calculated for ${}^{185}_{74}W$ and ${}^{203}_{80}Hg$ using the relativistic Hartree-Fock wave function for the K-shell electron. Both the effect of the phase-space sharing among three leptons (β^- particle, antineutrino, and emitted K-shell electron) and the exchange effect of two continuum electrons in the final state have been taken into account. The calculated results are compared with the previous theoretical calculations and with the experimental data.

II. THEORETICAL MODEL

When three leptons are ejected simultaneously, the differential K-electron shakeoff probability in β^- decay for emission of two electrons with the total energies W_1 and W_2 is given by

$$w_K(W_1, W_2)\,dW_1dW_2=\frac{G^2}{4\pi^5}|M_N|^2[P+Q-(PQ)^{1/2}] \times(W_K-W_1-W_2)^2p_1W_1dW_1p_2W_2dW_2, \qquad (1)$$

where

$$P=|M_A(W_1)|^2F(Z+1,\ W_2)S(W_2,\ W_K-W_1-W_2),$$
$$Q=|M_A(W_2)|^2F(Z+1,\ W_1)S(W_1,\ W_K-W_1-W_2).$$

Z is the atomic number of the parent nuclide, G the coupling constant of the weak interaction, p_1 and p_2 the mementa of two emitted electrons, M_N the energy-independent part of the nuclear matrix element, $M_A(W)$ the atomic matrix elemtnt for ejection of K-shell electron with the total energy W, $S(W_\beta,\ W_\nu)$ the shape factor for β-particle energy W_β and antineutrino energy W_ν, and $F(Z,\ W_\beta)$ the Fermi function for Z and W_β. The maximum energy available for K-electron ejection is given by $W_K=W_0+1-B_K$ where W_0 is the transition energy of β decay and B_K is the K-shell binding energy of the daughter atom. Throughout the present work the relativistic units are used ($\hbar=m_e=c=1$).

On the other hand, the probability for ordinary β decay is expressed as

$$P_\beta=\frac{G^2}{2\pi^3}|M_N|^2\int_1^{W_0}S(W_\beta,\ W_0-W_\beta)F(Z+1,\ W_\beta)(W_0-W_\beta)^2p_\beta W_\beta dW_\beta, \qquad (2)$$

where p_β is the momentum of the β particle corresponding to W_β.

From Eqs. (1) and (2), the total K-shell shakeoff probability per β^- decay is given by

$$P_K=\frac{1}{P_\beta}\int_1^{W_K} dW_1\int_1^{W_K-W_1} w_K(W_1,\ W_2)\,dW_2. \tag{3}$$

III. ATOMIC MATRIX ELEMENT

The atomic matrix element in Eq. (1) is defined by imperfect wave-function overlap:

$$M_A=<\phi_f(Z+1,\ W)\,|\,\phi_i(Z,\ K)>, \tag{4}$$

where $\phi_i(Z,\ K)$ is the wave function of a K-shell electron of the parent atom and $\phi_f(Z+1,\ W)$ is the continuum wave function of the total energy W in the Coulomb field of the daughter atom.

For the K-shell electron, we use the relativistic Hartree-Fock wave function in the Roothaan type.[9] In the relativistic Hartree-Fock-Roothaan (RHFR) model, the radial parts of the wave function for each orbital are expanded in terms of the Slater-type orbitals with nonintegral principal quantum number:

$$g(r)=\frac{1}{r}\sum_n \xi_n^{(1)}\varphi_n(r), \tag{5a}$$

$$f(r)=\frac{1}{r}\sum_n \xi_n^{(2)}\varphi_n(r), \tag{5b}$$

where $g(r)$ and $f(r)$ are the large and small parts of the radial wave functions, and $\xi_n^{(1)}$ and $\xi_n^{(2)}$ are the expansion coefficients. The Slater-type orbital is written by

$$\varphi_n(r)=(2\zeta_n)^{n'+1/2}[\Gamma(2n'+1)]^{-1/2}r^{n'}e^{-\zeta_n r}, \tag{6}$$

where $\Gamma(x)$ is the gamma function, and

$$n'=n+(\kappa^2-Z^2\alpha^2)^{1/2},\qquad n=0,\ 1,\ 2,\ \cdots\cdots. \tag{7}$$

Here κ is the κ-quantum number of the orbital and α is the fine structure constant. The values of the expansion coefficients and the orbital exponents are determined by the variational method so as to give the lowest stationary value for the energy and to satisfy the virial theorem for the energy.

On the other hand, the ejected electrons are expressed by the continuum-state solution of the Dirac equation with a central potential $V(r)$, which is determined by the inner- and outer-screening method. In this approximation, $V(r)$ is given by the sum of the Coulomb potential for the effective nuclear charge $Z_{eff}=Z-0.3$ and the difference between the measured K-shell binding energy and the *ideal* binding energy calculated from the hydrogenic model. According to Hock,[10] the potential thus obtained is a good approximation to the relativistic Hartree-Fock-Slater potential calculated by *Lu et al.*[11] in the vicinity of the K-shell radius. Then the continuum wave function is

the same as that in the hydrogenic model given in the text book of Rose[12] with modification of the nuclear charge and the kinetic energy.

The final expression for the atomic matrix element for ejection of the electron with total energy W in the present model is written by

$$M_A=C\left\{i\left[\frac{W-1}{2W}\right]^{1/2}\sum_n N(n)\,\xi_n^{(s)}L^{(+)}(n) + \left[\frac{W+1}{2W}\right]^{1/2}\sum_n N(n)\,\xi_n^{(i)}L^{(-)}(n)\right\}, \tag{8}$$

where

$$L^{(\pm)}(n)=(-i)^n u^{\gamma'-1}v^{\gamma+n+2}\Gamma(\gamma+\gamma'+n+1) \left[(\gamma'+iy)F(\gamma+\gamma'+n+1,\ \gamma'+1+iy;2\gamma'+1;u) \pm(1-iy/W)F(\gamma+\gamma'+n+1,\ \gamma'+iy;2\gamma'+1;u)\right], \tag{9}$$

$$C=(-i)^{\gamma+\gamma'+1}\frac{2\pi^{1/2}}{\Gamma(2\gamma'+1)}e^{\pi y/2}|\Gamma(\gamma'+iy)|,$$

$$N(n)=\left[(2\zeta)^5\Gamma(\gamma+1+2n-1)\right]^{-1/2}$$

with $\zeta=\alpha Z$, $\gamma'=[1-\alpha^2(Z+1)^2]^{1/2}$, $u=2p/(p-i\zeta)$, $v=2\zeta/(p-i\zeta)$, $y=\alpha(Z+1)W/p$. The function $F(a, b; c; x)$ is the Gauss-type hypergeometric fnction.

IV. NUMERICAL RESULTS AND DISCUSSION

We have calculated the K-electron shakeoff probabilities per β decay for ^{185}W and ^{203}Hg from Eq. (3) by the use of the atomic matrix element given in Eq. (8). The nuclear transition energy and the K-shell binding enrgy of the daughter atom are taken from the tables prepared by Lederer and Shirley.[13] All the calculations in the present work have been made on the FACOM M-200 computer of the Data Processing Center of Kyoto University.

In order to test the atomic matrix element in Eq. (8), the K-electron shakeoff probabilities have been calculated in the sudden approximation. In this approximation, the K-electron shakeoff process is assumed to occur in two step: β decay takes place as the first step and the K-shell electron emission is caused by the sudden change in the nuclear charge. The shakeoff probability is independent of the energy of β decay. Then the differential probability for emission of the electron with total energy W can be written by

$$P(W)\,dW=\frac{1}{\pi^2}|M_A|^2pW\,dW. \tag{10}$$

The calculated values of $P(W)\ dW$ for $_{80}Hg$ are plotted in Fig. 1 against the kinetic energy of the ejected electron. For comparison, the values with the hydrogenic wave function and those with the G-I wave function are also shown in the figure. It is interesting to note that the G-I wave function gives the probability in satisfactory agreement with the RHFR vaues in the low-energy region, while at high energies the G-I curve approaches to the hydrogenic values.

Table I. Comparison of the K-shell shakeoff probabilities in the sudden approximation

	Probability ($\times 10^{-4}$)	
	$_{74}W$	$_{80}Hg$
Hydrogenic	1.81	1.70
G-I	2.38	2.15
RHFR	2.12	2.03
Carlson *et al.*[a]	2.25	2.10

[a] Ref. 14.

The total K-shell ionization probability per β decay in the sudden approximation can be obtained by numerical integration of Eq. (10) with respect to W from 1 to ∞. The results are listed in Table I and compared with the values of the hydrogenic model, those of the G-I model, and the calculated values of Carlson *et al.*[14] In the model of Carlson *et al.*,[14] the probability is expressed in terms of overlap integrals between the bound-state wave functions only and the calculations have been performed with the relativistic Hartree-Fock-Slater wave functions. Therefore their values contain the contributions from the shakeup process and may be called the *K-hole production probability*.

It can be seen from the table that the present values are in good agreement with the values of Carlson *et al.* This fact indicates the validity of the present model. It is also reasonable that the present values are slightly smaller than the values of Carlson *et al.*, because the latter contain the contributions from the shakeup process. At the same time this means that the shakeup process plays a minor role in the K-hole production in β decay. The G-I model gives somewhat larger values than the results of Carlson *et al.* and the present model, but is in fair agreement with both values. This is due to the fact that as can be seen in Fig. 1 the G-I model yields the K-shakeoff probability in agreement with the RHFR values in the low-energy region, where the dominant contribution to the total probablity comes from. The main source of the error in the present model is attributed to the lack of orthogonality for the wave functions, becuase we use the different atomic potentils for the initial and final states. In order to estimate this effect, we have performed the similar calculations for the same atom by using the atomic matrix element $<\phi_i(Z, W)\,|\phi_f(Z, K)>$. The calculated results indicate that the error due to lack of orthogonality is less than 3% for ^{185}W and 5% for ^{203}Hg.

The final results for the K-shakeoff probabilities per β decay, including the effects of phase-space sharing and of the electron exchange are shown in Table II and compared with the recent experimental data. For comparison, the values of the hydrogenic model, those with the G-I wave functions, and the recent theoretical predictions of Law and Suzuki[15] are listed in the table.

The present results are slightly higher than the G-I values, but these two values are in satisfactory agreement with each other. This can be expected from the agreement between both models in Fig. 1 and Table I. It is also clear from the table that the many-electron effect plays an important role in the K-electron shakeoff probability.

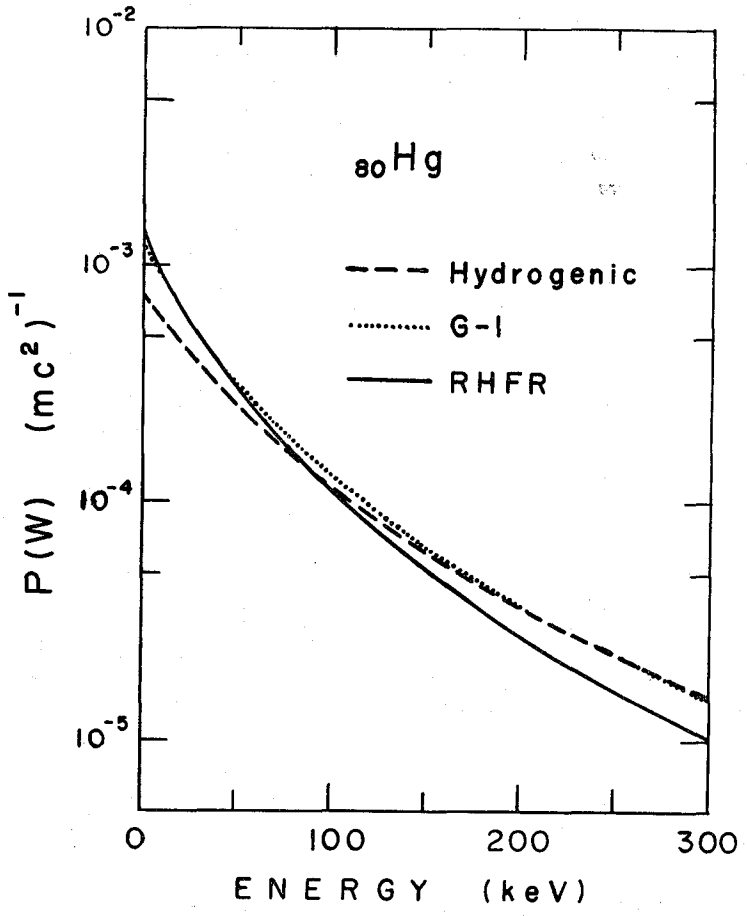

Fig. 1. The differential K-electron shakeoff probability of $_{80}Hg$ for emission of the electron with total energy W.

Table II. Comparison of the calculated K-shell shakeoff probabilities per β^- decay with the experimental data ($\times 10^{-4}$)

	$^{185}_{74}W$	$^{203}_{80}Hg$
Hydrogenic	0.383	0.0623
G-I	0.473	0.0843
RHFR	0.492	0.0957
OFDS[a]	0.78	0.13
Experiment	1.0±0.3[b]	0.11±0.035[d]
	1.0±0.2[c]	0.15±0.045[e]

[a] Law and Suzuki (Ref. 15)
[b] Campbell and Law (Ref. 16)
[c] Hansen and Parthasaradhi (Ref. 17)
[d] Bond *et al.* (Ref. 18)
[e] Thibaud *et al.* (Ref. 19)

However, the present values still somewhat smaller than the experimental data. Especially for ^{185}W, the calculated value is about a factor of 2 smaller than the measured values.

Recently Law and Suzuki[15] proposed a new model which is in good agreement with the experimental data. They used the optimized Dirac-Fock-Slater (ODFS) wave functions[20] and took into account the existence of the K-shell vacancy in the final state (the *relaxed-orbital approximation*). In their model, the K-shell vacancy produced by emission of the K-shell electron is considered to play an important role and the final atomic configuration is expressed as a doubly ionized ion, instead of a singly ionized atom in the ordinary *frozen-orbital* approximation. After β^- decay, the atomic number of the nucleus changes by one unit and the final atom has a vacancy in the outermost shell. The atomic potential for the final state is calculated for this state in the frozen-orbital approximation. In the relaxed-orbital approximation, an additional K-shell vacancy is introduced in the final atomic configuration and the final continuum wave function is calculated for this atomic potential.

It is easily seen that this approximation increases the K-shell ionization probability in the case of β^- decay and improves agreement with the experimental values. In general, K-electron shakeoff probability is proportional to the square of change in the effective nuclear charge.[21] If we use the Slater screening constant,[22] the effective nuclear charge for the K-shell electron in the ordinary atom can be written by $Z-0.3$. In the case of the frozen-orbital approximation, only the nuclear charge increases by one unit and the effective nuclear charge for the final state is $Z+0.7$. The difference in the effective nuclear charge is equal to one. On the other hand, in the relaxed-orbital approximation the effective charge for the K-shell electron in the final state is given by $Z+1$, and the change in the effective nuclear charge is equal to 1.3. This fact means that the K-electron shakeoff probability in the relaxed-orbital approximation is 1.69 times larger than the corresponding value in the frozen-orbital approximation. Multiplying this factor to the RHFR values in Table II, we obtain 8.31×10^{-5} for ^{185}W and 1.62×10^{-5} for ^{203}Hg. These values are in good agreement with the experimental results.

However, for the case of K-electron shakeoff process in β^+ decay the situation becomes contrary. In the relaxed-orbital approximation, the effective charge for the final state is $Z-1$ and the shakeoff probability is 0.49 times of that in the frozen-orbital approximation. This leads to the theoretical prediction considerably smaller than the experimental values. Practically the ODFS value for β^+ decay of ^{64}Cu calculated by Law and Suzuki[15] is 5.80×10^{-4}, which is a factor of 2 smaller than two experimental values $(13.2\pm0.8)\cdot10^{-4}$ by Schupp and Freedman[23] and $(13.3\pm1.1)\cdot10^{-4}$ by Scott.[24] Furthermore, in the relaxed-orbital approximation the shakeoff probability for β^+ decay of ^{64}Cu, $P_K(\beta^+)$, is smaller than that for β^- decay of the same nuclide, $P_K(\beta^-)$, while in the frozen-orbital approximation the former is slightly larger than the latter. The experimental result for the ratio of $P_K(\beta^+)/P_K(\beta^-)$ in ^{64}Cu is 1.19 ± 0.08,[23] and is in favor of the frozen-orbital approximation. These facts suggest that the agreement between the ODFS value and experiment for β^- is fortuitous.

In the previous work,[6,7] we have pointed out that the possible reasons for the discrepancy between theory and experiment can be ascribed to the existence of mechanisms other than the shakeoff process. Agreement between the RHFR values and

the values of Carlson *et al.*[14] in Table I indicates the smallness of the contribution from the shakeoff process.

Another possible mechanism is the direct-collision (DC) process. According to the simple estimation of Feinberg,[1] the contribution from this process is small, except for the case of very small transition energy. Intemann[25] made the nonrelativistic calculations for the DC process by the use of Coulomb Green function method and found that the contribution from this process is only about 12—15% of the total K-shell ionization probability.

On the other hand, we have shown[26] that the DC process is equivalent to internal conversion of the internal bremsstrahlung radiation accompanying β^- decay and estimated the probability based on some simplifying approximations. The obtained results indicate that the DC probability is comparable to the shakeoff probability and the sum of these two probabilities agrees well with the recent experimental values. Batkin *et al.*[27] have calculated the K-shell internal ionization probabilities during β^- decay in the unified model, including both shakeoff and DC processes. In their model, the calculations of the DC process is made in the manner similar to the method used by Intemann. However, their conclusion is opposite to the results of Intemann. The DC contribution is significant and amounts to 50% of the total ionization probability for ^{147}Pm and ^{203}Hg.

In conclusion, we have calculated the K-electron shakeoff probabilities in β^- decay by the use of the relativistic Hartree-Fock wave functions. The calculated results are in good agreement with the previous values obtained with the Greenland-Irvine wave functions. The theoretical predictions are still systematically smaller than the recent experimental data. The reason for the difference between the present theoretical calculations and the relaxed-orbital approximation is discussed. In order to clarify the discrepancy between theory and experiment, the relative contribution from the direct-collision process should be examined more carefully. The discrepancy between two calculations for the direct-collision process indicates that further theoretical studies on this proces is needed. More experimental data for the K-shakeoff probabilities in β^+ decay are also useful.

REFERENCES

(1) E. L. Feinberg, *J. Phys.* (*USSR*) **4**, 423 (1941).
(2) A. Migdal, *J. Phys.* (*USSR*), **4**, 449 (1941).
(3) See for example, M. S. Freedman, *Ann. Rev. Nucl. Sci.*, **24**, 209 (1974) ; R. J. Walen, and Ch. Briançon, "Atomic Inner Shell Processes," ed. by B. Crasemann, Academic Press, New York, (1975), p. 233.
(4) Y. Isozumi, S. Shimizu, and T. Mukoyama, *Nuovo Cimento*, **41a**, 1740 (1977).
(5) T. Mukoyama and S. Shimizu, *J. Phys. G: Nucl. Phys.*, **4**, 1509 (1978).
(6) P. T. Greenland and J. M. Irvine, *J. Phys. A: Math. Nucl. Gen.*, **5**, L 10 (1972).
(7) T. Mukoyama, *J. Phys. G: Nucl. Phys.*, **7**, 1675 (1981).
(8) F. Herman and S. Skillman, "Atomic Structure Calculations," Prentice-Hall, Englewood Cliffs, New Jersey, (1963).
(9) T. Kagawa, *Phys. Rev. A*, **12**, 2245 (1975).
(10) G. Hock, private communication.
(11) C. C. Lu, T. A. Carlson, F. B. Malik, T. C. Tucker, and C. W. Nestor, Jr., *Atomic Data*, **3**, 1 (1971).

(12) M. E. Rose, "Relativistic Electron Theory," Wiley, New York, (1961).
(13) C. M. Lederer and V. S. Shirley, "Table of Isotopes," John-Wiley & Sons, New York, (1978), 7 th edition.
(14) T. A. Carlson, C. W. Nestor, Jr., T. C. Tucker, and F. B. Malik, *Phys. Rev.*, **169**, 27 (1968).
(15) J. Law and A. Suzuki, *Phys. Rev. C*, **25**, 5141 (1982).
(16) J. L. Campbell and J. Law, *Can. J. Phys.*, **50**, 2451 (1972).
(17) H. H. Hansen and K. Parthasaradhi, *Phys. Rev. C*, **9**, 1143 (1974).
(18) A. Bond, O. P. Gupta, and A. Zide, *Phys. Rev. C*, **9**, 1529 (1974).
(19) T. H. Thibaud, Ch. Briançon, and R. J. Walen, *J. Physique*, **35**, L-89 (1974).
(20) I. Lindgren and A. Rosen, *Case Stud. At. Phys.*, **4**, 93 (1974).
(21) T. Mukoyama, *Acta Phys. Hung.*, **44**, 187 (1978).
(22) J. C. Slater, *Phys. Rev.*, **36**, 57 (1930).
(23) G. Schupp and M. S. Freedman, *Phys. Rev. C*, **21**, 348 (1980).
(24) R. D. Scott, *J. Phys. G: Nucl. Phys.*, **6**, 1427 (1980).
(25) R. L. Intemann, "Inner-Shell and X-Ray Physics of Atoms and Solids," ed. by D. J. Fabian, H. Kleinpoppen, and L. M. Watson, Plenum Press, New York, (1981), p. 295; and to be published.
(26) T. Mukoyama and G. Hock, *ATOMKI Közlemények*, **23**, 151 (1981).
(27) I. S. Batkin, I. V. Kopytin, Yu. G. Smirnov, and T. A. Churakova, *Sov. J. Nucl. Phys.*, **33**, 25 (1981).